PHASE-CHANGE TECHNIQUES FOR FINITE ELEMENT CONDUCTION CODES

INTRODUCTION

A method employing integral averaging techniques is proposed to aid conduction finite element code users in approximating multidimensional phase change problems such as: (a) liquid solidification under action of surface heat removal such as ice production or solidification of a casting, (b) thermal/chemical decomposition of a solid without removal of degraded material from the remaining virgin material such as charring of wood or reinforced plastics, (c) ablation of solids where the products of decomposition are removed on formation such as melting glass or subliming teflon. Of prime interest to the method is the determination of the amount of material solidified, decomposed, melted or sublimed and the location of the phase change interface as a function of time as it moves through the one-, two-, or three-dimensional finite element mesh. As the interface moves through each element, the energy involved in the phase change process and the difference in heat capacity and conductivity of two phases is accounted for. A method is also included to accommodate convective heat transfer at the moving phase change interface.

INTEGRAL AVERAGING TECHNIQUES

For a variable \( u \) which is dependent on temperature \( T \) as in Figure 1a, \( \bar{u} \), the average value of \( u \) in the interval from \( T_1 \) to \( T_3 \), is easily obtained by direct integration. With \( w = \int u dT \), the \( w \) vs \( T \) relationship would be of the form of Figure 1b. The average value of \( u \) in the interval can be determined as

\[
\bar{u}_{T_1,T_3} = \frac{dw}{dT}|_{T_1,T_3} = \frac{[w(T_3) - w(T_1)]}{(T_3 - T_1)}. \quad (1)
\]
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The defining symbol $\equiv$ in Equation (1) should be noted. The gradient term is not a usual derivative at every point between $T_1$ and $T_3$. It is, however, a special form that is defined to have only one value for the interval. An extension of the method that is useful is that if in the interval, $u$ is as illustrated in Figure 1c (where the integral from $T_2^-$ to $T_2^+$ has a known value), the average value of $u$ in the interval is still obtained directly by determining $w$ and then employing Equation (1).

For the first illustration given of $u$ vs $T$, a "series" type of average (analogous to series electrical circuit) of $u$ is defined as

$$u_{T_1,T_3} = 1/[(T_2-T_1)/u_1(T_3-T_1) + (T_3-T_2)/u_3(T_3-T_1)]. \quad (2)$$

This "series" average can also be obtained from the relationship

$$1/u_{T_1,T_3} = dw/dT |_{T_1,T_3} \equiv [w(T_3) - w(T_1)]/(T_3-T_1) \quad (3)$$

where

$$w(T_3) = w(T_1) + \int_{T_1}^{T_2} (1/u_1) \,dT + \int_{T_2}^{T_3} (1/u_3) \,dT. \quad (4)$$

If $T$ is dependent on a coordinate variable (say $x$), then $dw/dt$ can be expressed as $dw/dT = (dw/dx)/(dT/dx)$. For a linear triangular element where $T$ varies linearly throughout the element, the variables $dT/dx$ and $dT/dy$ are not difficult to determine. For a $u$ vs $T$ relationship of the form of Figure 1a, and a corresponding $w$ vs $T$ relationship of the form of Figure 1b, the $u$ variation as a function of position throughout the element is as illustrated in Figure 2a where the vertical distance represents the value of $u$ at any point. The dotted line is the projection of the element onto the x-y plane. The $w$ variation as a function of position throughout the element is illustrated in Figure 2b where the vertical distance represents the value of $w$ at any point.
The terms \( \frac{dw}{dx} \) in the \( x \) direction and \( \frac{dw}{dy} \) in the \( y \) direction within the element are defined to have only one value each for the whole element. They are obtained by passing a plane through the 3 points defining the values of \( w \) at each node as in Figure 2c and obtaining the gradients of the plane in the directions desired. With these values, \( \bar{u} \) and \( \bar{v} \) in each direction are then obtained. For a linear tetrahedral finite element, the concepts are the same although it is not possible to depict them with additional illustrations. The directional values of \( \bar{u} \) and \( \bar{v} \) can also be obtained for two- and three-dimensional linear isoparametric elements using the same methods.

PHASE CHANGE APPROXIMATION

Using these integral averaging techniques, a method is proposed which allows the conduction finite element code user to approximate phase change problems without having to change the mesh as the transient progresses. These techniques have been tried on a variety of problems where exact or approximate solutions are available. The results have been good but at best the method is only approximate.

Consider first one-dimensional linear elements. As a thermal transient progresses, a phase change interface may move through a particular element. The energy of the phase change and the difference in the conductivity of two phases must be accounted for within this element. With the conductivities of the two phases (\( k_a \) and \( k_b \)), and the interface position \( (x^*) \), the overall conduction resistance \( (R) \) to heat flow in the \( x \) direction within the element is

\[
R = \frac{(x^* - x_1)}{k_a A} + \frac{(x_2 - x^*)}{k_b A} \tag{5}
\]

where \( x_1 \) and \( x_2 \) are element nodal coordinates and \( A \) the cross
sectional area. From the following definition of the effective resistance \( R_e \),
\[
R_e = \frac{(x_2 - x_1)}{k_e A}
\]
the effective conductivity for the element \( (k_e) \) is
\[
k_e = \frac{(x_2 - x_1)}{[\left(\frac{x^* - x_1}{k_a} + \frac{x_2 - x^*}{k_b}\right)]}
\]
\( k_e \) is observed to be a series average, i.e., \( k_e = \bar{w} \) where \( w = \int (1/k) \, dt \). If \( k \) is some known function of temperature such as in Figure 3a (where \( T^* \) is the phase change temperature), the \( w \) vs \( T \) function can be determined.

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\[
ke = (x_2 - x_1)/[(x^* - x_1)/k_a + (x_2 - x^*)/k_b] \]

With the value of \( w \) and \( T \) at each node, the single valued terms \( dw/dx \) and \( dT/dx \) for the element are determined. The effective conductivity within the element is then
\[
l/k_e = (dw/dx)/(dT/dx).
\]
This approach will give the same result as previously obtained for \( k_e \). However, if \( dT/dx = 0 \), then \( dw/dx = 0 \) and the operation is not defined. In this case, \( k_e \) is \( k \) at the one \( T \) value in the element.

The volumetric heat capacity \( (pc) \) of the material is a function of temperature of the form illustrated in Figure 3b. The volumetric average value for \( pc \) in the element is
\[
pc = \left[\frac{(T^*-T_1)(pc_a+pc_a^*) + (T_2-T^*)(pc_b+pc_b^*)}{2(T_2-T_1)}\right]
\]
where \( pc_a \) and \( pc_b \) are the volumetric heat capacities for the two phases \( a \) and \( b \). By analogy then, \( pc \) is observed to be a regular average value, i.e., \( pc = \bar{w} \) where \( w = \int pc dT \). Thus
\[
pc = (dw/dx)/(dT/dx).
\]
If \( dT/dx = 0 \), \( dw/dx \) will \( = 0 \), in which case the operation is undefined and \( pc \) is the \( pc \) at the single value of \( T \) in the element.

In Reference 1 it is suggested that the \( pc \) vs \( T \) variation can be altered to effectively account for the energy of phase change when using a finite element "conduction only" type of code. This suggestion originates from the idea that in
thermodynamics—the quantity of enthalpy per unit volume \((e)\)
is related to volumetric specific heat as \(pc = de/dT\) where 
e\(e = \int pc \,dT\). Also, the volumetric heat of fusion or vaporization \((e^*)\) is a volumetric enthalpy "jump" across the phase change interface. If \(e\) is plotted as a function of \(T\) for a material, the relationship would be as shown in Figure 3c where the small region around \(T^* (2\Delta T^*)\) represents some small temperature range over which the phase change is assumed to take place. This \(\Delta T\) is not thought to be a sensitive parameter and it is recommended that it be chosen in the range of 1/100 to 1/1000 of the overall temperature difference seen in the problem. An effective volumetric specific heat is defined to include this enthalpy "jump" as

\[
pc_{\text{element}} = \frac{(de/dx)/(dT/dx)}{(de/dT)}. \tag{10}
\]

The use of such a definition not only approximates the volumetric average of \(pc\) in the element but also takes into account the effect of the latent heat term.

Using the technique described for a two-dimensional linear triangular element in which there is a conductivity discontinuity due to temperature variation in the element, the effective conductivity to be used for the element in the \(x\) direction is

\[
k_{x \text{ direction}} = \frac{1}{k_{\text{element}}} = \frac{(dw/dx)/(dT/dx)}{(dT/dx)} \tag{11}
\]

and with an obvious analogous equation for the \(y\) direction.

Even though the material may be isotropic, the presence of conductivity discontinuities as a function of temperature makes the material effectively anisotropic. The effective \(pc\) to be used in the element in the \(x\) direction is obtained with Equation (10) and with an obvious analogous equation for the \(y\) direction. However, in the standard heat conduction equation, directional \(pc\)'s have no meaning. This difficulty is circumvented by defining the effective \(pc\) to be used in the element as

\[
pc_{\text{element}} = \left[\frac{(de/dx)^2 + (de/dy)^2}{(dT/dx)^2 + (dT/dy)^2}\right]^{1/2}. \tag{12}
\]

This relationship is the effective value of \(de/dT\) for the element.

For a three-dimensional tetrahedral element in which there is a conductivity discontinuity due to temperature variation within the element, the effective conductivity to be used can be obtained from equations similar to those for a two-
Often phase change problems include convectively controlled heat transfer in the fluid at the solid-fluid interface. Numerically this is a difficult problem to approximate. The element which contains the phase change interface must take into account the combination of the conduction in the solid part and the convection in the fluid part. For the completely fluid elements which are close to the phase change element, the directional convection energy transfer to the interface must be accounted for. For fluid elements which are not close to the interface, the nodal temperatures are constrained to be at the fluid temperature $T_\infty$. For illustration purposes, let the conductivity of the solid phase be denoted as $k_S$. In the physical problem, the value of the conductivity in the fluid is usually of no computational interest since the heat transfer is only proportional to the convection coefficient $h$ and the temperature difference $\Delta T$ between the fluid temperature ($T_\infty$) and the surface temperature ($T^*$). The effective conductivity to be used for the liquid portion of the conduction finite element must reflect this convection information. For a one-dimensional element this is accomplished by requiring that the effective liquid conductivity ($k_{e,L}$) in the fluid portion of the phase change element be

$$k_{e,L} = h \frac{(T_\infty - T^*)}{(dT/dx)}$$  \hspace{1cm} (14)

In effect, this requires that the effective conduction flux in the liquid portion of the element ($k_{e,L}(dT/dx)$) be approximately the same as the imposed convective flux ($h (T_\infty - T^*)$). The term approximate is appropriate as the term $dT/dx$ to be used in obtaining $k_{e,L}$ is the last known value. The problem is non-linear and successive approximations must be employed. The overall effective conductivity in the complete phase change element is obtained as a series average of $k_S$ and $k_{e,L}$ as per Equation (8) where

$$w = \int_{T_0}^{T^*} (1/k_S) dT + \int_{T^*}^{T} \frac{dT/dx}{h (T_\infty - T^*)} dT.$$  \hspace{1cm} (15)

For adjacent elements which are completely in the liquid region, the effective solid conductivity that is to be used must reflect the convection process being approximated. It might be assumed that this could be accomplished by choosing the effective conductivity in the element as per Equation (14). However, such is not the case for an all fluid element. Detailed calculations indicate that the process of choosing $k_{e,L}$
for the next calculation based only on the last known value of \( \frac{dt}{dx} \) is divergent. A process that works well is a relative error reduction technique which approaches the result of Equation (14). For example, if the resulting heat flux is 20% low, the value of \( k_e \) is increased by 20%. Fluid elements that are not close to the phase change element may be constrained to be at \( T_\infty \). One way to determine if the element is close or not is to initially constrain all liquid nodes to be at \( T_\infty \) (except for the nodes on the initial phase change interface), then as the solidification progresses, check within each element and if any one of the nodal temperatures of that element is \( \leq T_\infty \), remove the \( T_\infty \) constraint from all nodes of that element. This process assures that at least the fluid nodes between the phase change element and the adjacent fluid element are not constrained to be \( T_\infty \)..

In the two- and three-dimensional problems of this type, the following additional considerations must also be made: (a) in the phase change elements, the convective heat flux vector (perpendicular to the phase change interface) in the fluid side must be decomposed into its cartesian components. The respective value in each direction is then used to set up the \( w \) vs \( T \) relationship from which the effective directional conductivity is determined; (b) in each fluid element the convective heat flux vector must also be decomposed into its cartesian components and these respective values used to determine the effective conductivities to be employed in each direction.

INTERELEMENT STEP CHANGE IN CONDUCTIVITY

Solidification of an infinite slab of liquid for a case where an exact analytical solution is available is considered to illustrate the effect of the choice of Equation (8) to define the effective \( k \) of a material undergoing a phase change. An exact analytical solution to this problem is given in Reference 4. The problem there considered is the initially liquid infinite slab \((x > 0)\) at a constant temperature \( T_i \), which is greater than the fusion temperature \( T^* \). For time \( t \geq 0 \), the surface at \( x = 0 \) is maintained at a constant temperature, \( T_w \), that is lower than \( T^* \). At time \( t = 0 \), a change of phase occurs at \( x = 0 \); at time \( t > 0 \) the phase change occurs at the phase boundary, that is expressed by \( x = \beta \sqrt{t} \), where \( \beta \) is the phase boundary function. The finite element result of choosing various effective-\( k \) relationships to account for the piecewise continuous \( k \) function through the element containing the phase change front on the proportionality factor \( \beta \) between the penetration depth and the square root of the time was determined using typical water-ice properties. Choosing \( k \) based on the average temperature in the element resulted in a 10% high \( \beta \) value. Choosing a \( k \) value based on a regular average value technique resulted in a \( \beta \) that was 5% high. The best results were obtained with the series average method which gave results within 2% of the correct value.
INTERELEMENT STEP CHANGE IN HEAT CAPACITY

Solidification of a liquid in a quarter space \((x, y \geq 0)\) for a case where an exact analytical solution is available is considered to illustrate the choice of Equation (13) to define the effective \(\rho c\) of a material undergoing phase change. An exact analytical solution to this problem for a special set of conditions is given in Reference 5. The problem considered is the initially liquid quarter-space \((x, y \geq 0)\) at a constant temperature, \(T_1\), which is greater than the fusion temperature, \(T^*\). For time \(t \geq 0\), the surfaces \(x = 0\) and \(y = 0\) are maintained at a constant temperature, \(T_w\), that is lower than \(T^*\). At time \(t = 0\), a change of phase occurs along the surfaces \(x = 0\) and \(y = 0\); at time \(t > 0\), the phase change occurs at the phase boundary, that is expressed by \(y = f(x, t)\). The conductivity values of the two phases were chosen to be the same. The finite element results of choosing various effective \(\rho c\) relationships to account for the phase change phenomena along the line \(y = x\) were determined. Using the average of the two directional \(\rho c\) terms of Equation (10) resulted in a 5% error in the intersection of the free boundary function and the line \(y = x\). However, using the \(\rho c\) values determined from Equation (13) gave results within 1% of the solution of Reference 5.

INTERNAL SOLID TO LIQUID CONVECTIVE HEAT TRANSFER

The uniform convective cooling and accompanying solidification of a plane semi-infinite body \((x > 0)\) where the heat transfer between the liquid and solid occurs by convection is considered to illustrate the method suggested to include internal convection effects. A solution to this problem for a special set of conditions is given in Reference 3. The problem considered there is an initially liquid infinite slab \((x > 0)\) at a constant temperature \(T_1\), which is greater than the fusion temperature \(T^*\). For time \(t \geq 0\), the ambient air temperature at \(x < 0\) is maintained at a constant temperature \(T_a\) that is lower than \(T^*\). Heat transfer between the air and the liquid (or solid) occurs by convection \((h)\) at \(x = 0\). Also, at the solid-liquid interface, convection \((h_i)\) controls the heat transfer. In Figure 4 is shown the solidification depth as a function of the other pertinent parameters. The finite element results were obtained relying on the method previously outlined.

INTERNAL SOLID TO GAS CONVECTIVE HEAT TRANSFER

Ablation of a semi-infinite solid \((x > 0)\) where the thermally degraded or melted material is removed as it forms is considered to further illustrate the method suggested to include internal convection effects. The general problem of predicting material ablation requires consideration of complex material-degradation processes and material/environment interactions.
However, various approximate analyses are available for predicting general behavior during quasi-steady ablation of materials that degrade in depth. The one to be used for comparison purposes from Reference 6 is a simplified quasi-steady solution considering in-depth reactions but no internal transpiration or property changes in the decomposition layer (considered to be a surface). In the problem under consideration, it is assumed that a semi-infinite homogeneous solid \( x \geq 0 \) initially at constant temperature \( T_i \) is suddenly (at \( t \geq 0 \)) heated by convection so that eventually a phase change occurs (at \( t^* \) when the surface temperature reaches \( T^* \)) and the new phase is removed upon formation. The preablition time \( t^* \) is the time required for the surface to attain the decomposition temperature \( T^* \). At some time in excess of \( t^* \), the ablation velocity \( v \) approaches a constant value \( v_s \) and the surface recedes at a constant rate. For the following dimensionless groups, set at the values indicated,

\[
(h(T_a-T^*)/e^*)(t^*/a_s)^{1/2} = 1 \quad \text{and} \quad (T_a-T^*)(T^*-T_i) = 0.35
\]

the penetration depth \( \xi \) as a function of time is shown in Figure 5. The finite element results obtained are also shown.

CONCLUSIONS

Finite element conduction codes may be used to approximate phase change problems using the techniques described in this paper. A variety of such problems have been approximated with various multidimensional conduction finite element codes and the results compare favorably with exact solutions or other approximate solutions. The great utility of the methods presented is that they may be applied in one, two, or three dimensions for very complex problems (including convective...
heat transfer at the phase change interface) with difficult geometries where in general exact solutions do not exist. Reference 2 gives additional details of the techniques discussed in this paper.

REFERENCES